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Study of Superconductivity in Li based binary alloys of alkali metals using HFP Pseudopotential Technique

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ABSTRACT

By using technique of Harrison's First Principle Pseudopotential we studied superconductivity in binary alloys of Li with other alkali metals. Historically HFP Pseudopotential method has been rarely used. Unique opportunity is explored to use HFP Pseudopotential technique to study SSP like T_c, λ *and* μ^* *of alkali metal alloys of Li. SSP of Li and Li based binary alloys of alkali metals at varying concentration 0.9 to 0.1 were computed through McMillan's formalism (1968). V-S form of screening is used in present work for obtaining SSP of Li based alkali metal binary alloys. As a variant SSP are studied using three different forms of eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C). Comparison of present values of SSP with available experimental and theoretical findings by other scholars are highly encouraging. Further, results computed in our present work will enrich the data bank for SSP of alkali-alkali binary alloy.*

Key Words : Li, Alloys, Alkali, Li based binary alloys etc.

I. INTRODUCTION

In its history, the condensed matter physics has revealed an amazingly diverse range of materials, properties and phenomena. Superconductivity is a unique and powerful phenomenon of nature that occurs in certain materials below a critical temperature. It is a special type of phase transition that does not involve any crystallographic or order-disorder phase transition but a totally new kind of phase transition. The phenomenon of superconductivity remains an active area of research by both experimental and theoretical physicists. A lot has happened in the span of more than hundred years since Kamerlingh Onnes (1911) discovered this delightfully strange phenomenon of superconductivity in Hg. W. Meissner (1932) in his research found a large number of binary alloys and compounds to be superconducting. It was also found that when alloying a non-superconducting metal with a superconducting one Tc may be increased.

Also, Matthias (1957, 1973) from his study concluded that metals with Z<2 do not exhibit superconducting nature; Hence, alkali metals (Z=1) are non-superconducting. But, unpredictably, Cs was reported as, first alkali metal with superconducting properties under high pressure J. Wittig, (1970); W. Buckel and W. Weber (1982).

J.C. Boettger and S.B. Trickey (1985) in his study also indicated band narrowing and gap-widening in Li under extreme compression, i.e. drastic deviations from free electron behaviour. Later, Lin and Dunn (1986) reported that above 20 GPa the lightest alkali metal, Li, exhibits both a positive resistivity derivative dρ/dP and some type of phase transition near 5 K, perhaps a superconducting transition. The discovery of superconducting alkali metal fullerides came in 1991

when Robert Haddon and Bell Labs announced that K3C60 had been found to superconduct at 18 K.

II. Technique and Formulism Used

To realize the objective to investigate superconducting state parameter in Li based alkali-alkali binary alloy, HFP pseudopotential technique (1966) is employed. The main objective of our present work is to divulge the salient feature of the alloys under investigation. As HFP pseudopotential technique is more rigorous and having sound theoretical background; the various interacting potentials have arrived in this technique through fundamental considerations employing quantum mechanical and statistical mechanics approach along with Poisson's equation. However, in previous paper Sunil et al (2017) optimized model potential theory was used to study electrical resistivity of molten Na, K alloy; the HFP pseudopotential technique has been acknowledged to be more rigorous than the model potential technique and being used in this present work. Moreover, HFP pseudopotential technique is also free from arbitrariness in choosing a model or its parameter i.e., no arbitrary adjustable parameter has been introduced and no arbitrary model has been proposed.

2.1 Elemental Information of Alkali metals:

In this subsection we have presented some of the elemental information of alkali metals which is also used as an input values in our computation are tabulated below in Table – 1 below:

Table – 1

Properties	**Li**	**Na**	**K**	**Rb**	**Cs**
Atomic number (A)	3	11	19	37	55
Most common isotopes	Li-7 (92.41%) Li-6 (7.59%)	Na-23	K-39(93.26) K-40(0.01) K-41(6.73)	Rb-85(72.17) Rb-87(27.83)	Cs-133
Crystal Structure	bcc	bcc	bcc	bcc	bcc
Melting point	453.69 K	373.15	338.15	313.15	303.15
Boiling point	1615.15 K	1156.15	1032.15	961.15	944.15
θ_D	352 K	157 K	59.4 K	54 K	40 K
Atomic weight (M)	6.94	22.99	39.10	85.47	140.12
m_b	1.19	1.00	0.94	1.00	0.98
m^*	2.20	1.26	1.24	1.25	1.43
Z	1	1	1	1	1
Z^*	1.03	1.10	1.14	1.17	1.19
r_c a.u	1.4541	2.0234	2.6370	2.7885	3.5913
Atomic volume(Ω_0)	153.3334	278.0259	531.1665	650.7534	809.1086
Density (ρ)g/cm^3	0.534	0.971	0.862	1.532	1.873
Fermi wave vector(k_F)	0.5780	0.4740	0.3820	0.3570	0.3320

Fermi energy(E_F)		4.76	3.20	2.12	1.81	1.57
βRydbergs-a.u.		29.1	27.0	31.5	32.9	44.9
ω_L (10^{-4}a.u.)		14.700	5.586	3.344	2.021	1.507
ω_T (10^{-4}a.u.)		8.085	3.161	1.580	1.014	0.779
V-S constants	A	1.00714	1.07783	1.16730	1.19750	1.23459
	B	0.29857	0.28554	0.27051	0.26573	0.26010

Values for alkali-alkali binary alloy was computed using Vegard Rule-

$$\alpha_{A_xB_{1-x}} = x\alpha_A + (1-x)\alpha_B \quad (1)$$

2.2 McMillan Formulism for SSP of metals and alloys

The study of the relation between microscopic theory and observed superconducting transition temperature T_c was made by McMillan (1968)

i. Expression for transition temperature (T_c) :

By inverting Zero-temperature and thus using tunnelling conductance Eliasberg theory McMillan and Rowell (1969) determine $\alpha^2(\omega)\,F(\omega)$and μ^*. T_c was determined from the interaction parameters $\alpha^2(\omega)\,F(\omega)$ and μ^*. Because the gap $\Delta(\omega)$ vanishes at T_c , this becomes a linear equation for infinitesimal function $\Delta(\omega)$. The condition that a nonzero solution exists determines the value of T_c .

The formula for superconducting transition temperature as a function of coupling constants for the electron-phonon and Coulomb interactions with an accuracy of ~1% was derived as –

$$T_c = \frac{\Theta_D}{1.45}\ exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\,\lambda)}\right] \quad (2)$$

McMillan (1968) used this Debye Θ for characteristic phonon frequency.

Dyne (1972) later introduced $\frac{\langle\omega\rangle}{1.20}$ in place of $\frac{\Theta_D}{1.45}$ and rewrites the equation as-

$$T_c = \frac{\langle\omega\rangle}{1.20}\ exp\left[-\frac{1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\,\lambda)}\right] \quad (3)$$

The formulation of McMillan has been re-analysed, particularly for the case of strong coupling superconductors, by Allen and Dynes (1975), Nowotny (1976), (1976) and Leavens (1976).

Equation (3) is used in our present work for calculation of T_c of alkali metals and alkali-alkali binary alloys.

ii. **Expression for electron-phonon coupling strength** (λ) :

From the definition of electron-phonon coupling strength (λ) McMillan (1968) presented the following expression –

$$(\lambda) = 2\int \frac{d\omega\, \alpha^2(\omega)\, F(\omega)}{\omega} = \frac{N(0)\langle g^2\rangle}{2M\langle\omega^2\rangle} \tag{4}$$

where

$\langle\omega^2\rangle$ is an average of the square of the phonon frequency.

Equation (4) when appropriately evaluated in the plane wave approximation for the scattering on the Fermi surface, Jain S. C. and Kachhawa C. M (1980) yields

$$\lambda = \frac{m_b}{4\pi^2 k_F M\, N < \omega^2 >} \int_0^{2k_F} q^3 |w(k,q)|^2 dq \tag{5}$$

where,

w(k, q) the screened Pseudopotential form factor

M is ionic mass

Z is the valence of the corresponding metallic ions

m_b is the band mass of electron

$< \omega^2 >$ is the average square phonon frequency of metal

q is the momentum transfer

N is the ion number density

Same expression is also used by Sharma et al. (2003). We further simplified the expression as below -

As N can be expressed as-

$$N = \frac{1}{\Omega_0} = \frac{k_F^3}{3\pi^2 Z} \tag{6}$$

Putting this value in above equation (4), we have

$$\lambda = \frac{3\, m_b\, Z}{4\, k_F^4\, M\, <\omega^2>} \int_0^{2k_F} q^3\, |w(k,q)|^2\, dq \qquad (7)$$

Taking ,

$$\eta = \frac{q}{k_F}$$

we have

$$dq = k_F\, d\eta$$

Thus,

at $q = 0$; $\eta = 0$, and, at $q = 2k_F$; $\eta = 2$

Changing the limits of integration, we get

$$\lambda = \frac{3\, m_b\, Z}{4\, M\, <\omega^2>} \int_0^{2} \eta^3\, |w(k,\eta)|^2\, d\eta \qquad (8)$$

In present work we have used this simplified expression for computing the value of λ for alkali metals and alkali-alkali binary alloys.

iii. **Expression for Coulomb pseudopotential (μ^*) :**

Making use of the theoretical equations and experimental results McMillan (1968) empirically extract an expression for the Coulomb pseudopotential (μ*) Various simplified expressions of the Coulomb pseudopotential (μ*) by different authors in the past. In our present work we have used the simplified expression of Gajjar et al. (2004)

$$\mu^* = \frac{\frac{m_b}{\pi k_F} \int_0^1 \frac{dX}{X\varepsilon^*(X)}}{1 + \frac{m_b}{\pi k_F} \ln\left(\frac{E_F}{10\,\theta_D}\right) \int_0^{2k_F} \frac{dX}{q\varepsilon^*(X)}} \qquad (9)$$

where

$$X = \frac{q}{2\, k_F} \qquad (10)$$

Sharma et al. (2003) have also used this formula with $\frac{k_F^2}{20\,\theta_D}$ in place of $\frac{E_F}{10\,\theta_D}$, we have used $\frac{E_F}{K_B\theta_D}$ instead. And further simplified the expression as below-

$$\mu^* = \frac{\frac{m_b}{\pi k_F}\int_0^1 \frac{dX}{X\varepsilon^*(X)}}{1+\frac{m_b}{\pi k_F}\ln\left(\frac{E_F}{K_B\theta_D}\right)\int_0^{2k_F}\frac{dX}{q\varepsilon^*(X)}} \quad (11)$$

As, we have taken

$$\eta = \frac{q}{k_F}$$

From equation (9), we have

$$\eta = 2X$$

or, $d\eta = 2\,dX$

Further,

$$\text{at } X = 0;\ \eta = 0 \text{ and, at } X = 1;\ \eta = 2$$

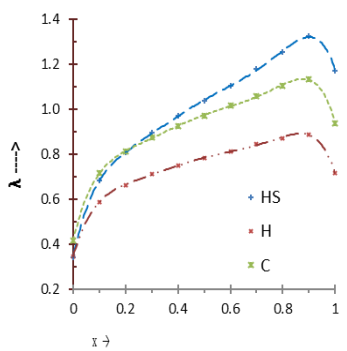
Hence, changing the limits of integration, we get

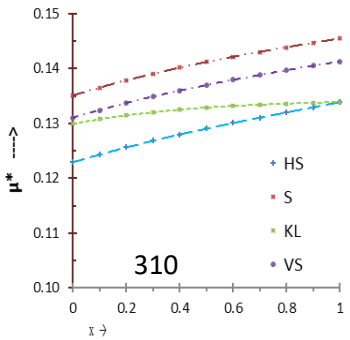
$$\mu^* = \frac{\frac{m_b}{\pi k_F}\int_0^2 \frac{d\eta}{\eta\varepsilon^*(\eta)}}{1+\frac{m_b}{\pi k_F}\ln\left(\frac{E_F}{K_B\theta_D}\right)\int_0^{2}\frac{d\eta}{\eta\varepsilon^*(\eta)}} \quad (12)$$

Above simplified expression is also used in our previous work Sunil and M.M. Khan (2017) to compute Coulomb pseudopotential (μ*) of alkali metals and alkali-alkali binary alloys at different concentration.

III. Computation of SSP:

SSP of Li and Li based binary alloys of alkali metals Li_x-Na_{1-x}, Li_x-K_{1-x}, Li_x-Rb_{1-x} and Li_x-Cs_{1-x}, where x is the concentration factor of first alkali metal, are investigated for varying concentration at x=0.9-0.1 were computed through McMillan's formalism (1968). Computed values of SSP like $\mathbf{T_c}$, λ and μ^* of alkali metal alloys of Li are plotted in Figure 1- 4 Below:





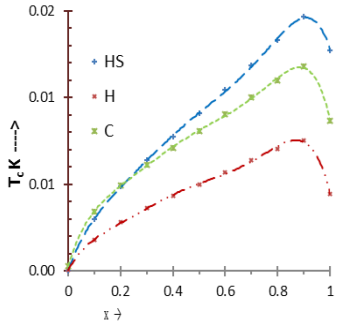


Fig 1: SSP of $Li_x - Na_{1-x}$ ($x = 0.9\ to\ 0.1$) using V-S exchange function with eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C) near melting point.

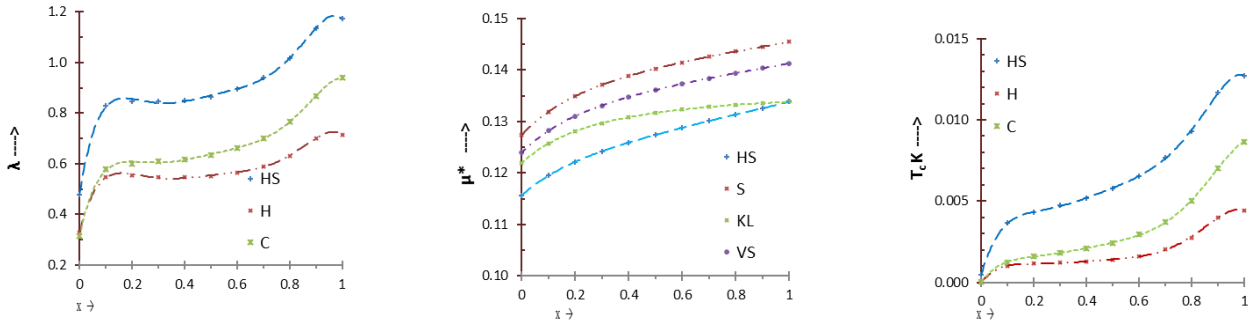


Fig 2: SSP of $Li_x - K_{1-x}$ (x = 0.9 *to* 0.1) using V-S exchange function with eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C) near melting point.

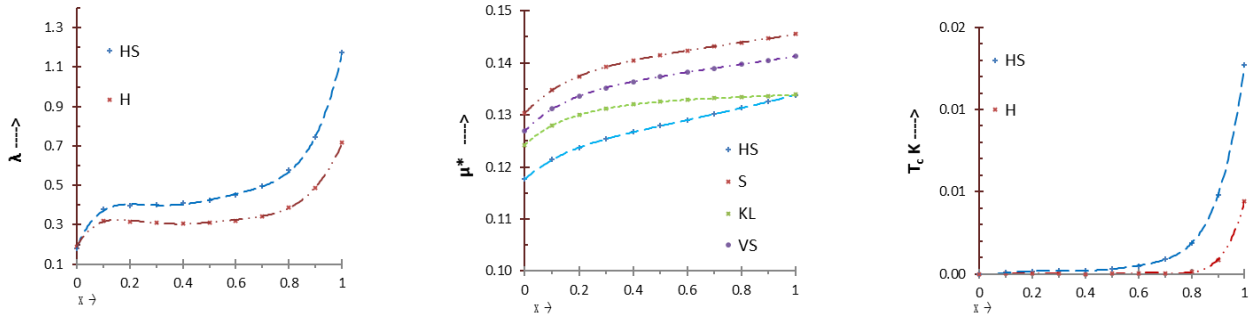


Fig 3: SSP of $Li_x - Rb_{1-x}$ (x = 0.9 *to* 0.1) using V-S exchange function with eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C) near melting point.

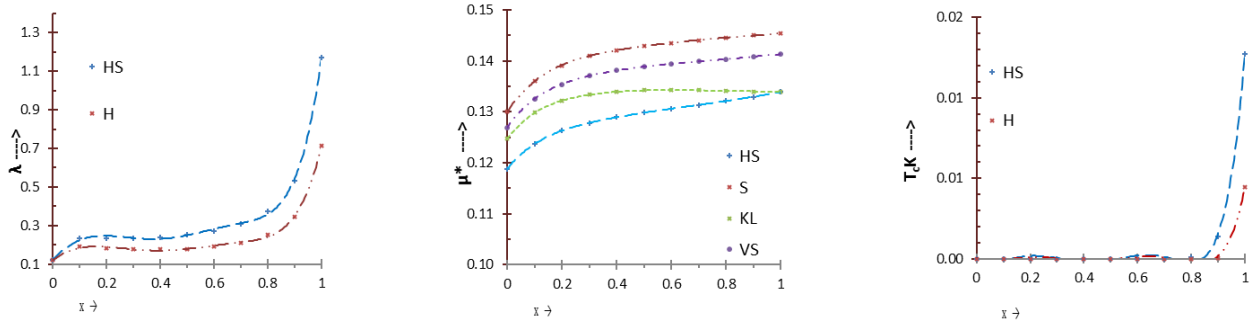


Fig 4: SSP of $Li_x - Cs_{1-x}$ ($x = 0.9\ to\ 0.1$) using V-S exchange function with eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C) near melting point.

IV. Result And Discussion

The result obtained in present work are comparable in fair agreement with other theoretical data set of Vohra et al. (2006) Gazzar et al. (2004) Sharma and Sharma (1983) Morel and Anderson Jain et al. (1980) Allen (1999) Allen (1969) Rajput et al. (1969) McMillan (1968). Results are encouraging, and the SSP of Lithium based alkali binary alloys has been obtained with adequate accuracy by using the HFP pseudopotential technique.

In our present investigation we used four different form of local field correlation function Hubbard – Sham (1965), Shaw (1967), Kleinmann – Langreth (1968) and Vashishta – Singwi (1972) to incorporate screening effect while computing μ^*. From previous work Sunil et. al (2017) we perceived V-S form of screening to be most suitable. Thus, V-S form of screening is used in present work for obtaining SSP of Li based alkali metal binary alloys. As a variant SSP are studied using three different forms of eigenvalues of Herman-Skillman (HS), Hafner (H) and Clementi (C).

Since very little data is available for the SSP of the A_x-B_{1-x} alkali-alkali binary alloys therefore it is difficult to draw any special remarks. However, Comparison of presently value with scarcely available experimental and theoretical findings is highly encouraging. Further, results computed in our present work will enrich the data bank for SSP of alkali-alkali binary alloy and our observation to the present investigation may provide guideline to future research in this field.

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